

Fractional exclusion statistics in disordered systems

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Abstract

We develop a model based on the fractional exclusion statistics, applicable to disordered interacting particle systems. Here the species represent elementary volumes in an $(s + 1)$ -dimensional space, formed by the direct product between the s -dimensional space of positions and the quasiparticle energy axis. The model is particularly suitable for systems with localized states. Using the fermionic, bosonic and Wu perspectives of the FES formalism, we present the properties of systems with repulsive screened Coulomb interactions. We analyze the case of the homogeneous system, as well as a few test cases with non-uniformities in the local density of states. The particle density is determined and the margin (charging) effects are pointed out. In addition, peculiar deviations observed in the temperature dependence of the heat capacity and entropy are found, in accordance with the several degrees of disorder considered.

1. Introduction

The concept of fractional exclusion statistics (FES) was introduced by Haldane [1] and the statistical properties of FES systems were calculated independently by Wu [2] and Isakov [3].

The FES was applied to quasiparticle excitations at lowest Landau level in the fractional quantum Hall effect, spinon excitations in a spin- $\frac{1}{2}$ quantum antiferromagnet [1, 2], Bose and Fermi systems described in the thermodynamic Bethe ansatz [3, 4, 5, 6], excitations [1] or motifs of spins [7, 8] in spin

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chains, elementary volumes obtained by coarse-graining in the phase-space of a system [3, 9, 10, 11, 12, 13], etc.

More recently, a stochastic method for the simulation of the time evolution of FES systems was introduced [14], as a generalization of a similar method used for Bose and Fermi systems [15], and the general FES formalism was amended to include the change of the FES parameters at the change of the particle species [11, 16, 17, 18]. This makes of FES a general formalism which is able to describe interacting particle systems as ideal gases of quasiparticles [19, 20].

A FES system consists of a countable set of species, indexed by $i, j = 0, 1, 2, \dots$. Each species contains a finite number of single-particle states and particles, denoted by G_i and N_i , respectively. The number of states in the species depend on the number of particles. For small variations of the number of particles around some reference distribution, $\{N_i\}_{i=0,1,\dots}$, the number of states changes by

$$\delta G_i = - \sum_j \alpha_{ij} \delta N_j, \quad (1)$$

where by δN_i we denote the particle variations and α_{ij} 's are called the FES parameters [1].

The FES parameters must satisfy certain rules [16], namely if we split an arbitrary species, j , into a number of sub-species, j_0, j_1, \dots , then all the parameters α_{kl} , with both, k and l different from j , remain unchanged, whereas the rest of the parameters must satisfy the relations:

$$\alpha_{ij} = \alpha_{ij_0} = \alpha_{ij_1} = \dots, \text{ for any } i, i \neq j \quad (2a)$$

$$\alpha_{ji} = \alpha_{j_0i} + \alpha_{j_1i} + \dots, \text{ for any } i, i \neq j \quad (2b)$$

$$\alpha_{jj} = \alpha_{j_0j_0} + \alpha_{j_1j_0} + \dots = \alpha_{j_0j_1} + \alpha_{j_1j_1} + \dots = \dots \quad (2c)$$

These rules are satisfied by the ansatz [11, 13],

$$\alpha_{ij} = \alpha_{ij}^{(e)} + \alpha_i^{(s)} \delta_{ij}, \quad (3a)$$

where the parameters $\alpha_{ij}^{(e)}$, called the “extensive” parameters, are proportional to G_i ,

$$\alpha_{ij}^{(e)} \equiv a_{ij} G_i. \quad (3b)$$

The parameters $\alpha_i^{(s)}$ refer to only one species and do not depend on G_i .

The number of microscopic configurations compatible to a given distribution of particles on species, $\{N_i\}$, is

$$W^B(\{N_i\}) = \frac{(G_i + N_i - 1)!}{N_i!(G_i - 1)!} \quad \text{and} \quad W^F(\{N_i\}) = \frac{G_i!}{N_i!(G_i - N_i)!}, \quad (4)$$

if the particles are bosons and fermions, respectively.

If for each species of particles, say species i , we associate an energy, ϵ_i , and a chemical potential μ_i then the equilibrium particle distribution, $n_i \equiv N_i/G_i$, is obtained by maximizing the partition function,

$$\mathcal{Z}^{(P)} \equiv \sum_{\{N_i\}} \left\{ W^{(P)}(\{N_i\}) \exp \left[\beta \sum_j (\epsilon_j - \mu_j) N_j \right] \right\}, \quad (5)$$

with respect to the distribution $\{N_i\}$, taking into account that the G_j 's vary with $\{N_i\}$ according to (1). In Eq. (5) P is used instead of “B” or “F” from Eqs. (4) and $\beta = 1/(k_B T)$ is the inverse temperature.

The maximization of $\mathcal{Z}^{(P)}$ with the conditions (1) gives

$$\beta(\mu_i - \epsilon_i) + \ln \frac{1 \pm n_i^P}{n_i} = \pm \sum_j \alpha_{ji} \ln[1 \pm n_j^P]. \quad (6a)$$

where the all the upper “+” signs are for bosons and the lower “−” signs are for fermions.

If one uses the ansatz (3), Eq. (6a) becomes [13]

$$\beta(\mu_i - \epsilon_i) + \ln \frac{[1 \pm n_i^P]^{1-\alpha_i^{(s)}}}{n_i^P} = \pm \sum_j G_j a_{ji} \ln[1 \pm n_j^P]. \quad (6b)$$

In FES, a system of fermions with a set of parameters, $\{\alpha_{ij}\}$, may be interpreted as a system of bosons with the parameters $\{\alpha_{ij} + \delta_{ij}\}$ and vice-versa, a system of bosons of parameters $\{\alpha_{ij}\}$ may be interpreted as a system of fermions with the parameters $\{\alpha_{ij} - \delta_{ij}\}$. Therefore it is more natural to refer to the Bose and Fermi *formulations*, rather than to *bosons* and *fermions*.

The most used formulation of FES is the one employed by Wu in Ref. [2], which will be denoted here by “W”. To see how this is related to the Bose formulation we define the number of states in the absence of particles in the

system, $G_i^{\text{W}} \equiv G_i + \sum \alpha_{ij} N_j$, and a new particle population, $n_i^{\text{W}} \equiv N_i / G_i^{\text{W}}$. Then the n_i^{W} 's are determined in two steps. First one solves the system

$$(1 + w_i) \prod_j \left(\frac{w_j}{1 + w_j} \right)^{\alpha_{ji}} = e^{(\epsilon_i - \mu)/k_{\text{B}} T}, \quad (7a)$$

to determine the w_i 's, and then the n_i^{W} 's are calculated from

$$\sum_j (\delta_{ij} w_j + \alpha_{ij} G_j^{\text{W}} / G_i^{\text{W}}) n_j = 1. \quad (7b)$$

Comparing Eqs. (6a) and (7a) we observe that $w_i \equiv 1/n_i^{\text{B}}$.

In Refs. [19, 20] one of us have shown that FES is the natural description of an interacting particle system as a system of ideal quasiparticles. In this paper we exemplify this procedure on disordered systems of interacting localized particles. This method may find applications in glassy systems such as the Coulomb glasses and systems of bosons trapped in optical lattices.

The structure of the paper is as follows. In Section 2 we introduce our model, in which species are elementary volumes in the $(s + 1)$ -dimensional space formed by the direct product between the s -dimensional space of positions, Ω , and the energy axis, ϵ or $\tilde{\epsilon}$. These species are related by FES parameters, which we calculate. The formalism is then applied to homogeneous systems (mean-field approximation) and the FES parameters are calculated for a repulsive screened Coulomb potential. In Section 3 we apply our formalism on a few test cases, which are one-dimensional periodic systems with several degrees of disorder.

2. Model and formalism

The particles are localized on random sites in a solid s -dimensional matrix. The positions of the sites are denoted by \mathbf{r}_I , $I = 1, 2, \dots, N_0$, where N_0 is the total number of sites. We assume that the wavefunctions of the particles do not overlap and the total energy of the system is

$$E = \sum_I \epsilon_{\mathbf{r}_I} n_{\mathbf{r}_I} + \frac{1}{2} \sum_{I,J} V_{\mathbf{r}_I \mathbf{r}_J} n_{\mathbf{r}_I} n_{\mathbf{r}_J}. \quad (8)$$

where $\epsilon_{\mathbf{r}_I}$ is the energy and $n_{\mathbf{r}_I}$ is the occupation number of the site I ; the total particle number is $N = \sum_I n_{\mathbf{r}_I}$.

We shall work in the continuous limit, so we define the density of sites, $\sigma(\mathbf{r}, \epsilon) \equiv \sum_I \delta^s(\mathbf{r} - \mathbf{r}_I) \delta(\epsilon - \epsilon_{\mathbf{r}_I})$, and the particle density, $\rho(\mathbf{r}, \epsilon) \equiv \sum_I \delta^s(\mathbf{r} - \mathbf{r}_I) \delta(\epsilon - \epsilon_{\mathbf{r}_I}) n_{\mathbf{r}_I}$. The average particle population in the $(s+1)\text{D}$ volume $\delta\Omega \times \delta\epsilon$ is defined as $n(\mathbf{r}, \epsilon) = [\int_{\delta\Omega} d^s \mathbf{r} \int_{\delta\epsilon} d\epsilon \rho(\mathbf{r}, \epsilon)] / [\int_{\delta\Omega} d^s \mathbf{r} \int_{\delta\epsilon} d\epsilon \sigma(\mathbf{r}, \epsilon)]$, where we assume that the volume is large enough, so that $\int_{\delta\Omega} d^s \mathbf{r} \int_{\delta\epsilon} d\epsilon \sigma(\mathbf{r}, \epsilon) > 0$. In these notations the total energy of the system (8) becomes

$$E = \int_{\Omega} d^s \mathbf{r} \int_{\epsilon_{\min}}^{\epsilon_{\max}} \epsilon \rho(\mathbf{r}, \epsilon) d\epsilon + \frac{1}{2} \int_{\Omega} d^s \mathbf{r} \int_{\Omega} d^s \mathbf{r}' \times \int_{\epsilon_{\min}}^{\epsilon_{\max}} d\epsilon \int_{\epsilon_{\min}}^{\epsilon_{\max}} d\epsilon' \rho(\mathbf{r}, \epsilon) \rho(\mathbf{r}', \epsilon') V_{\mathbf{r}\mathbf{r}'} \quad (9)$$

where Ω is total the volume of the system and $[\epsilon_{\min}, \epsilon_{\max}]$ is the interval in which ϵ takes values, with $\epsilon_{\min} \geq 0$.

We shall assume that $\epsilon_{\min} = 0$, $\epsilon_{\max} \gg k_B T$ (where k_B is the Boltzmann constant and T is the temperature) and the interaction energy depends only on the distance between the sites, i.e. $V_{\mathbf{r}_I \mathbf{r}_J} \equiv V(|\mathbf{r}_I - \mathbf{r}_J|)$. Because $\epsilon_{\max} \gg k_B T$, we shall take $\epsilon_{\max} = \infty$.

For concreteness, we analyze only Fermi system, but the formalism can be easily extended to bosons.

To apply FES, we have to divide the system into species. We do this by coarse-graining the parameters space of the system, $\Omega \times \epsilon$, into the elementary volumes, $\delta\Omega_{\xi} \times \delta\epsilon_i$. By the lower case Greek letters, e.g. $\xi = 0, 1, \dots$, we identify the spatial volume and by the lower case Latin letters, e.g. $i = 0, 1, \dots$, we identify the energy intervals, $\delta\epsilon_i \equiv [\epsilon_i, \epsilon_{i+1}]$. We have $\epsilon_0 = 0$.

We identify a species either directly, by $\delta\Omega_{\xi} \times \delta\epsilon_i$, or by the subscripts, (ξ, i) . We assume that each elementary volume, $\delta\Omega_{\xi}$, is centered at \mathbf{r}_{ξ} and contains a large enough number of sites and particles to justify the application of the statistical methods and, in particular the Stirling approximation for the logarithms of factorial numbers. In each of the volumes, say $\delta\Omega_{\xi}$, we have a distribution of sites, $\mathbf{r}_I \in \delta\Omega_{\xi}$, of energies $\epsilon_{\mathbf{r}_I}$. Under the assumption that the number of sites is large enough, the set of energies $\{\epsilon_{\mathbf{r}_I}\}_{\mathbf{r}_I \in \delta\Omega_{\xi}}$ form a (quasi)continuous distribution along the ϵ axis, with a density $\sigma_{\xi}(\epsilon) \equiv \int_{\delta\Omega_{\xi}} \sigma(\mathbf{r}, \epsilon) d^s \mathbf{r}$. The number of states in the species (ξ, i) is then $G_{\xi i} = \sigma_{\xi}(\epsilon_i) \delta\epsilon_i$ and the number of particles is $N_{\xi i} = \sigma_{\xi}(\epsilon_i) \delta\epsilon_i n(\mathbf{r}_{\xi}, \epsilon_i) \equiv \delta\Omega_{\xi} \delta\epsilon_i \rho(\mathbf{r}_{\xi}, \epsilon_i)$. We shall use the notations $\rho_{\xi}(\epsilon) \equiv \rho(\mathbf{r}_{\xi}, \epsilon)$ for the particle density and $\rho_{\xi} \equiv \int d\epsilon \rho(\mathbf{r}_{\xi}, \epsilon)$ for the *volume* particle density.

We define the quasiparticle energies, $\tilde{\epsilon}_{\mathbf{r}_I}$, in a similar way as in Ref. [12,

21], by

$$\tilde{\epsilon}_{\mathbf{r}_I} = \epsilon_{\mathbf{r}_I} + \sum_{\tilde{\epsilon}_{\mathbf{r}_J} < \tilde{\epsilon}_{\mathbf{r}_I}} V(|\mathbf{r}_I - \mathbf{r}_J|) n_{\mathbf{r}_J}. \quad (10)$$

Because of the identity $E = \sum_I \tilde{\epsilon}_{\mathbf{r}_I} n_{\mathbf{r}_I}$, the thermodynamics of the quasiparticle gas follows identically the thermodynamics of the original system.

In the continuous limit, Eq. (10) becomes

$$\tilde{\epsilon}_{\mathbf{r}_I} = \epsilon_{\mathbf{r}_I} + \int_{\Omega} d^s \mathbf{r} \int_0^{\epsilon_{\mathbf{r}_I}} d\epsilon V(|\mathbf{r}_I - \mathbf{r}|) \sigma(\mathbf{r}, \epsilon) n(\mathbf{r}, \epsilon), \quad (11)$$

which is similar to Eq. (5) of Ref. [12], except that here we have an extra integral over \mathbf{r} .

We have a new parameters space, $\Omega \times \tilde{\epsilon}$, in which, by construction, $\tilde{\epsilon}_{\min} = \epsilon_{\min} = 0$ and $\tilde{\epsilon}_{\max} = \epsilon_{\max} = \infty$. Using Eq. (11) we obtain the new DOS,

$$\tilde{\sigma}[\mathbf{r}, \tilde{\epsilon}(\epsilon)] = \sigma(\mathbf{r}, \epsilon) \left| \frac{d\tilde{\epsilon}}{d\epsilon} \right|^{-1} = \frac{\sigma(\mathbf{r}, \epsilon)}{\left| 1 + \int_{\Omega} d^s \mathbf{r}' V(|\mathbf{r} - \mathbf{r}'|) \sigma(\mathbf{r}', \epsilon) n(\mathbf{r}', \epsilon) \right|}. \quad (12)$$

Assuming that Eq. (11) defines a one-to-one function $\tilde{\epsilon}(\epsilon)$ – which may also be inverted to $\epsilon(\tilde{\epsilon})$ – we split the space $\Omega \times \tilde{\epsilon}$ into species, $\delta\Omega_{\xi} \times \delta\tilde{\epsilon}_i$, as we did with $\Omega \times \epsilon$, in such a way that $\tilde{\epsilon}_i \equiv \tilde{\epsilon}(\epsilon_i)$ for any i and each species contains $G_{\xi i}$ states and $N_{\xi i}$ particles, as before.

By direct application of the procedure of Ref. [12, 21] to this interaction potential and particle species we obtain the FES parameters

$$\begin{aligned} \alpha_{\xi i; \eta j} &= \left[\delta_{ij} \sigma_{\xi}(\epsilon_i) + \theta(i - j) \delta\epsilon_i \frac{d\sigma_{\xi}(\epsilon_i)}{d\epsilon_i} \right] V(|\mathbf{r}_{\xi} - \mathbf{r}_{\eta}|) \\ &\equiv \left[\delta_{ij} \delta\Omega_{\xi} \sigma(\mathbf{r}_{\xi}, \epsilon_i) + \theta(i - j) \delta\epsilon_i \delta\Omega_{\xi} \frac{\partial \sigma(\mathbf{r}_{\xi}, \epsilon_i)}{\partial \epsilon_i} \right] V(|\mathbf{r}_{\xi} - \mathbf{r}_{\eta}|) \end{aligned} \quad (13)$$

where the first doublet, (ξi) , specifies the species in which the number of states changes, whereas the second doublet, (ηj) , specifies the species in which the number of particle changes; $\theta(k)$ is the step function, $\theta(k > 0) = 1$ and $\theta(k \leq 0) = 0$. The manifestation of the FES parameters given by Eq. (13) for a system with $\sigma(\mathbf{r}, \epsilon) \equiv \sigma(\mathbf{r})$, i.e. independent of ϵ , between species of the same quasiparticle energies is represented in Fig. 1.

We observe that the FES parameters (13) obey the rules (2) [16] and define a new ansatz, which is a generalization of the ansatz (3) [13].

2.1. Equilibrium thermodynamics

Since we have fermions in the systems, we employ the Fermi formulation [13] to calculate the equilibrium thermodynamics. Plugging the α parameters (13) into the equations (6) we get

$$0 = \beta(\mu - \tilde{\epsilon}_i) + \ln \frac{1 - n^F(\mathbf{r}_\xi, \tilde{\epsilon}_i)}{n^F(\mathbf{r}_\xi, \tilde{\epsilon}_i)} + \sum_{\eta j} \alpha_{\eta j; \xi i} \ln[1 - n^F(\mathbf{r}_\eta, \tilde{\epsilon}_j)]. \quad (14)$$

In the continuous limit, Eq. (14) becomes

$$\begin{aligned} 0 = & \beta(\mu - \tilde{\epsilon}) + \ln \frac{1 - n^F(\mathbf{r}, \tilde{\epsilon})}{n^F(\mathbf{r}, \tilde{\epsilon})} + \int_{\Omega} d^s \mathbf{r}' V(|\mathbf{r}' - \mathbf{r}|) \sigma[\mathbf{r}', \epsilon(\tilde{\epsilon})] \ln[1 - n^F(\mathbf{r}', \tilde{\epsilon})] \\ & + \int_{\Omega} d^s \mathbf{r}' V(|\mathbf{r}' - \mathbf{r}|) \int_{\tilde{\epsilon}}^{\infty} d\tilde{\epsilon}' \left. \frac{\partial \sigma(\mathbf{r}', \epsilon)}{\partial \epsilon} \right|_{\epsilon(\tilde{\epsilon}')} \ln[1 - n^F(\mathbf{r}', \tilde{\epsilon}')]. \end{aligned} \quad (15)$$

In the bosonic formulation, as we mentioned above, $\alpha_{\xi i; \eta j}^B \equiv \delta_{\xi \eta} \delta_{ij} + \alpha_{\xi i; \eta j}$, and the dimension of the species is the number of available states, $G_{\xi i}^B \equiv G_{\xi i} - N_{\xi i} + 1$ (we used the notation $G_{\xi i}^B$ to avoid confusion with the number of states in the species, $G_{\xi i}$). This changes also the definition of the population to $n^B(\mathbf{r}_\xi, \epsilon_i) \equiv N_{\xi i} / G_{\xi i}^B \equiv n(\mathbf{r}_\xi, \tilde{\epsilon}_i) / [1 - n(\mathbf{r}_\xi, \tilde{\epsilon}_i)]$. Plugging the new quantities into Eqs. (6) we obtain the system of equations for $n^B(\mathbf{r}_\xi, \epsilon_i)$:

$$0 = \beta(\mu - \tilde{\epsilon}_i) + \ln \frac{1 + n^B(\mathbf{r}_\xi, \tilde{\epsilon}_i)}{n^B(\mathbf{r}_\xi, \tilde{\epsilon}_i)} - \sum_{\eta j} \alpha_{\eta j; \xi i}^B \ln[1 + n^B(\mathbf{r}_\eta, \tilde{\epsilon}_j)] \quad (16)$$

and in the continuous limit,

$$\begin{aligned} 0 = & \beta(\mu - \tilde{\epsilon}) + \ln \frac{1 + n^B(\mathbf{r}, \tilde{\epsilon})}{n^B(\mathbf{r}, \tilde{\epsilon})} - \int_{\Omega} d^s \mathbf{r}' V(|\mathbf{r}' - \mathbf{r}|) \sigma[\mathbf{r}', \epsilon(\tilde{\epsilon})] \ln[1 + n^B(\mathbf{r}', \tilde{\epsilon})] \\ & - \int_{\Omega} d^s \mathbf{r}' V(|\mathbf{r}' - \mathbf{r}|) \int_{\tilde{\epsilon}}^{\infty} d\tilde{\epsilon}' \left. \frac{\partial \sigma(\mathbf{r}', \epsilon)}{\partial \epsilon} \right|_{\epsilon(\tilde{\epsilon}')} \ln[1 + n^B(\mathbf{r}', \tilde{\epsilon}')]. \end{aligned} \quad (17)$$

In Wu's formulation [2] the dimension of the species is $G_{\xi i}^W = G_{\xi i} + \sum_{\eta j} \alpha_{\xi i; \eta j} N_{\eta j} \equiv G_{\xi i}^B + \sum_{\eta j} \alpha_{\xi i; \eta j}^B N_{\eta j}$ and $n^W(\mathbf{r}_\xi, \epsilon_i) \equiv N_{\xi i} / G_{\xi i}^W$. The equilibrium population is calculated from

$$(1 + w_{\xi i}) \prod_{\eta, j} \left(\frac{w_{\eta j}}{1 + w_{\eta j}} \right)^{\alpha_{\eta j; \xi i}^B} = e^{(\epsilon_{\xi, i} - \mu) / kT}, \quad (18a)$$

and

$$\sum_{\eta,j} (\delta_{\xi\eta} \delta_{ij} w_{\eta j} + \beta_{\xi i, \eta j}) n_{\eta j}^W = 1, \quad (18b)$$

where $\beta_{\xi i, \eta j} = \alpha_{\xi i, \eta j}^B G_{\eta j}^W / G_{\xi i}^W \equiv \delta_{\xi\eta} \delta_{ij} + \alpha_{\xi i, \eta j} G_{\eta j}^W / G_{\xi i}^W$. We observe again that $w_{\xi i} \equiv (n_{\xi i}^B)^{-1}$.

Having the quasiparticle populations, we can calculate any thermodynamical quantity. The internal energy of the system is

$$U(T, \mu) = \sum_I n_{\mathbf{r}_I} \tilde{\epsilon}_{\mathbf{r}_I} = \sum_{\xi i} n^F(\mathbf{r}_\xi, \tilde{\epsilon}_i) G_{\xi i}^F \tilde{\epsilon}_i \equiv \sum_{\xi i} n^B(\mathbf{r}_\xi, \tilde{\epsilon}_i) G_{\xi i}^B \tilde{\epsilon}_i \equiv \sum_{\xi i} n^W(\mathbf{r}_\xi, \tilde{\epsilon}_i) G_{\xi i}^W \tilde{\epsilon}_i \quad (19)$$

or, in the continuous limit,

$$U(T, \mu) = \int_{\Omega} d^s \mathbf{r} \int_0^\infty d\tilde{\epsilon} \tilde{\sigma}^P(\mathbf{r}, \tilde{\epsilon}) n^P(\mathbf{r}, \tilde{\epsilon}) \tilde{\epsilon} \equiv \int_{\Omega} d^s \mathbf{r} \int_0^\infty d\tilde{\epsilon} \tilde{\rho}(\mathbf{r}, \tilde{\epsilon}) \tilde{\epsilon}, \quad (20)$$

where $P = F, B, W$ and $\tilde{\sigma}^F(\mathbf{r}, \tilde{\epsilon})$ is given by Eq. (12). The other two densities of states are $\tilde{\sigma}^B(\mathbf{r}, \tilde{\epsilon}) \equiv \tilde{\sigma}^F(\mathbf{r}, \tilde{\epsilon}) - \tilde{\rho}(\mathbf{r}, \tilde{\epsilon})$ and $\tilde{\sigma}^W(\mathbf{r}, \tilde{\epsilon})$ and all satisfy the relation $\tilde{\rho}(\mathbf{r}, \tilde{\epsilon}) \equiv \tilde{\sigma}^F(\mathbf{r}, \tilde{\epsilon}) n^F(\mathbf{r}, \tilde{\epsilon}) \equiv \tilde{\sigma}^B(\mathbf{r}, \tilde{\epsilon}) n^B(\mathbf{r}, \tilde{\epsilon}) \equiv \tilde{\sigma}^W(\mathbf{r}, \tilde{\epsilon}) n^W(\mathbf{r}, \tilde{\epsilon})$.

We shall use the notation $\tilde{\rho}_\xi(\tilde{\epsilon}) \equiv \tilde{\rho}(\mathbf{r}_\xi, \tilde{\epsilon})$ for the quasi-particle density in Ω_ξ , at quasiparticle energy $\tilde{\epsilon}$, and $\tilde{\rho}_\xi \equiv \int d\tilde{\epsilon} \tilde{\rho}(\mathbf{r}, \tilde{\epsilon})$ for the *volume* quasi-particle density. One should note that $\tilde{\rho}_\xi \equiv \rho_\xi$ by definition.

In order to define the DOS $\tilde{\sigma}^W(\mathbf{r}, \tilde{\epsilon})$ we have to define the densities of the FES parameters [11, 13], $a_{\mathbf{r}\tilde{\epsilon}; \mathbf{r}'\tilde{\epsilon}'}$, by

$$\alpha_{\xi i, \eta j} = a_{\mathbf{r}_\xi \tilde{\epsilon}_i; \mathbf{r}_\eta \tilde{\epsilon}_j} \delta \epsilon_i \delta \Omega_\xi \quad (21a)$$

where

$$a_{\mathbf{r}_\xi \tilde{\epsilon}_i; \mathbf{r}_\eta \tilde{\epsilon}_j} = \left[\delta(\tilde{\epsilon}_i - \tilde{\epsilon}_j) \sigma(\mathbf{r}_\xi, \epsilon_i) + \theta(\tilde{\epsilon}_i - \tilde{\epsilon}_j) \frac{\partial \sigma(\mathbf{r}_\xi, \epsilon_i)}{\partial \epsilon_i} \right] V(|\mathbf{r}_\xi - \mathbf{r}_\eta|) \quad (21b)$$

Using Eqs. (21) we write $\tilde{\sigma}^W(\mathbf{r}, \tilde{\epsilon}) = \tilde{\sigma}^F(\mathbf{r}, \tilde{\epsilon}) + \int_{\Omega} d^s \mathbf{r}' \int_0^\infty d\tilde{\epsilon}' a_{\mathbf{r}\tilde{\epsilon}; \mathbf{r}'\tilde{\epsilon}'} \tilde{\rho}(\mathbf{r}', \tilde{\epsilon}')$.

Similarly, the total particle number is

$$N(T, \mu) = \int_{\Omega} d^s \mathbf{r} \int_0^\infty d\tilde{\epsilon} \tilde{\sigma}^P(\mathbf{r}, \tilde{\epsilon}) n^P(\mathbf{r}, \tilde{\epsilon}) \equiv \int_{\Omega} d^s \mathbf{r} \int_0^\infty d\tilde{\epsilon} \tilde{\rho}(\mathbf{r}, \tilde{\epsilon}). \quad (22)$$

The heat capacity and the entropy of the system are

$$C_V = \left(\frac{\partial E}{\partial T} \right)_N = \frac{\partial U(T, \mu)}{\partial T} - \frac{\partial U(T, \mu)}{\partial \mu} \frac{\partial N(T, \mu)}{\partial T} \left(\frac{\partial U(T, \mu)}{\partial \mu} \right)^{-1} \quad (23)$$

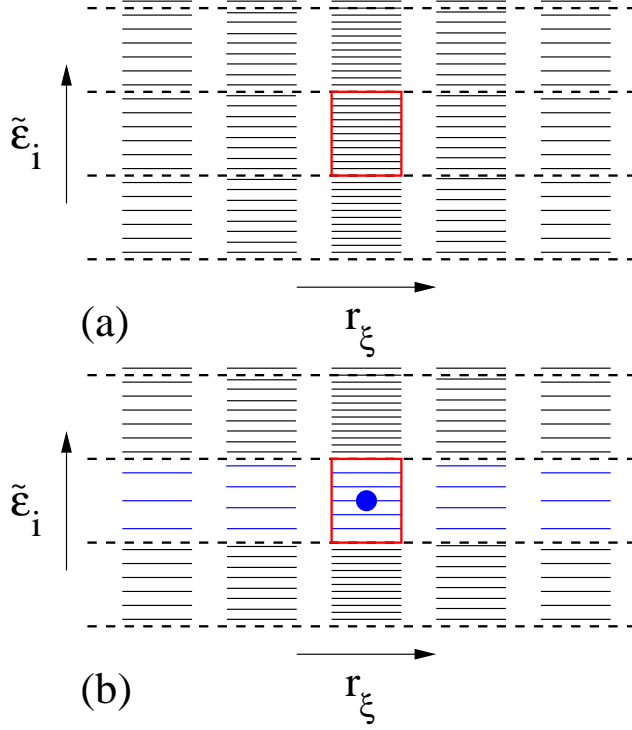


Figure 1: Partitioning of real space and quasiparticle energy axis. Upon inserting an extra particle in species (ξ, i) , the numbers of available states in all species (η, i) are changed.

and

$$S = k_B \ln(W^P), \quad (24)$$

respectively, and they satisfy the equation

$$C_V = T \left(\frac{\partial S}{\partial T} \right)_N. \quad (25)$$

2.2. Homogeneous system

If $\sigma(\mathbf{r}, \epsilon) \equiv \sigma_\Omega(\epsilon)$ is independent of \mathbf{r} and if we impose periodic boundary conditions or ignore the effect of the surfaces (deep inside the solid), then both, $n(\mathbf{r}, \epsilon)$ and $\tilde{\sigma}(\mathbf{r}, \tilde{\epsilon})$, are independent of \mathbf{r} and in the Eqs. (15) and (17) we can perform the integrals over Ω to obtain an effective FES parameter,

$$\alpha_{\text{eff}}(\tilde{\epsilon}) = \sigma_\Omega[\epsilon(\tilde{\epsilon})] I_V \left[1 + \int_{\tilde{\epsilon}}^{\infty} d\tilde{\epsilon}' \frac{\partial \sigma_\Omega(\epsilon)}{\partial \epsilon} \Big|_{\epsilon(\tilde{\epsilon}')} \right], \quad (26)$$

where

$$I_V = \int_{\Omega} d^s \mathbf{r}' V(|\mathbf{r}' - \mathbf{r}|). \quad (27)$$

Plugging α_{eff} back into Eqs. (15) and (17) we get the equations

$$\beta(\tilde{\epsilon} - \mu) = -\ln \frac{[1 - n^{\text{F}}(\mathbf{r}, \tilde{\epsilon})]^{1-\alpha_{\text{eff}}}}{n^{\text{F}}(\mathbf{r}, \tilde{\epsilon})} = \ln \frac{[1 + n^{\text{B}}(\mathbf{r}, \tilde{\epsilon})]^{1+\alpha_{\text{eff}}}}{n^{\text{B}}(\mathbf{r}, \tilde{\epsilon})} \quad (28)$$

3. Applications

We exemplify the formalism above by assuming a two-particle screened potential of the general form

$$V(r; \gamma, \lambda) = \kappa \frac{\exp(-r/\lambda)}{r^\gamma}, \quad (29)$$

where $r = |\mathbf{r} - \mathbf{r}'|$. In particular, if $\gamma = 1$, we have the usual screened Coulomb and Yukawa type potentials. Such systems exhibit standard thermostatistical behavior if $d/\gamma < 1$ [22] and the interactions are classified as short ranged. If $d/\gamma \geq 1$ the systems obey *non-extensive* thermodynamics, i.e. quantities like total energy are not extensive due to the long range interactions.

To remove the singularity at the origin that appear in the integrals over V in Eqs. (15), (17) and (27), we introduce a cut-off at radius R_0 , below which the potential remains constant – $V(r) = V(R_0) \equiv V_0$ for $r < R_0$. With this assumption, for a homogeneous system,

$$I_V = \frac{2\pi^{\frac{s}{2}}}{\Gamma(\frac{s}{2})} \int_0^\infty dr r^{s-1} V(r) = I_{V1} + I_{V2}, \quad (30)$$

where

$$\begin{aligned} I_{V1} &\equiv \frac{2\pi^{\frac{s}{2}}}{\Gamma(\frac{s}{2})} \int_0^{R_0} dr r^{s-1} V(r) = \frac{\pi^{\frac{s}{2}}}{\Gamma(\frac{s}{2} + 1)} R_0^s V_0 \\ I_{V2} &\equiv I_V - I_{V1} = \frac{2\pi^{\frac{s}{2}}}{\Gamma(\frac{s}{2})} \kappa \sigma \lambda^{s-\gamma} \Gamma\left(s - \gamma, \frac{R_0}{\lambda}\right). \end{aligned} \quad (31)$$

Here $\Gamma(s, x) = \int_x^\infty t^{s-1} e^{-t} dt$ is the upper incomplete gamma function.

For a screened Coulomb-type interaction in a s -dimensional system ($s = 1, 2, 3$), the term I_{V2} can be expressed as:

$$\begin{aligned} I_{V2}^{1D} &= 2\kappa\sigma E_1(R_0/\lambda) \\ I_{V2}^{2D} &= 2\pi\kappa\sigma \lambda \exp\left(-\frac{R_0}{\lambda}\right) \\ I_{V2}^{3D} &= 4\pi\kappa\sigma \lambda(R_0 + \lambda) \exp\left(-\frac{R_0}{\lambda}\right), \end{aligned} \quad (32)$$

where $E_1(z)$ is the exponential integral,

$$E_1(z) = \int_z^\infty \frac{e^{-t}}{t} dt = \int_1^\infty \frac{e^{-zt}}{t} dt. \quad (33)$$

3.1. Application to one-dimensional disordered interacting systems

To illustrate some peculiar thermodynamical properties of interacting disordered systems we apply our FES formalism to 1D disordered systems with periodic boundary conditions. The physical space is partitioned into N_R subvolumes on the coordinate axis and N_E segments on the energy axis, which define a total number of $N_R \times N_E$ species. The periodic boundary conditions are imposed using the minimum image convention, i.e. the interaction drops at a distance equal to half the length of the repetitive unit.

For simplicity we shall assume in the following that $\sigma(\mathbf{r}, \epsilon)$ [and $\sigma_\xi(\epsilon)$] are independent of ϵ , so we shall simplify the notation of the DOS to $\sigma(\mathbf{r})$ (and σ_ξ). In this case the FES parameters (13) simplify to

$$\alpha_{\xi i; \eta j} = \delta_{ij} \sigma_\xi(\epsilon_i) V(|\mathbf{r}_\xi - \mathbf{r}_\eta|) \equiv \delta_{ij} \delta \Omega_\xi \sigma(\mathbf{r}_\xi, \epsilon_i) V(|\mathbf{r}_\xi - \mathbf{r}_\eta|) \quad (34)$$

which is diagonal in the indices i and j .

For our 1D system we apply a spatial partitioning such that $\Omega_\xi \equiv R_\xi = 1$ and we take the cut-off distance, R_0 , to be half of the species dimension, i.e. $R_0 = R_\xi/2$. Furthermore, we set $V(R_\xi) = 1$, which implies $V(R_0) = 2$. Under these assumptions we rewrite the FES parameters in Eq. (34) as:

$$\begin{aligned} \alpha_{\xi i; \xi i} &= \sigma_\xi(\epsilon_i) V_0 R_\xi \\ \alpha_{\xi i; \eta j} &= \delta_{ij} \sigma_\xi(\epsilon_i) (V_0/2) R_\xi^2 / |\mathbf{r}_\xi - \mathbf{r}_\eta| \quad \text{for } i \neq j. \end{aligned}$$

The quasiparticle densities $\tilde{\rho}_\xi(\tilde{\epsilon})$, $\tilde{\rho}_\xi$ can be found in any of the descriptions aforementioned (F, B, W) by solving the corresponding nonlinear system (15), (17) or (18). The solution is found iteratively using gradient descent

– as implemented by GSL – starting from an initial guess solution. Since the thermodynamical quantities of interest should be obtained for a given particle number N rather than for a given μ , an extra loop is introduced so that the corresponding chemical potential is found in agreement with the normalization relation (22).

We consider a system with repulsive screened Coulomb interactions, parameterized by $\gamma = 1$ and $\lambda = 3R_\xi$. For the partition of the physical space and the coarse graining on the energy axis we take $N_R = 20$ and $N_E = 50$, respectively. The system contains a number of $N = N_R E_F \sigma$ particles, where the $E_F = 1$ is the Fermi energy. In this way we set up the energy scale. We also assume that $k_B = 1$.

Two particularly transparent examples of an inhomogeneous system are obtained by introducing a dip or a peak in the density of states of a homogeneous system. More concretely, we pick one sub-volume ζ for which the density of states is half or twice the reference (constant) value of the other sub-volumes, respectively: $\sigma_\xi = 1.0$ for any $\xi \neq \zeta$ and $\sigma_\zeta = 0.5$ (“dip” case) or 2.0 (“peak” case). For symmetry reasons we have considered $N_R + 1$ sub-volumes. Figure 2 depicts the particle densities for the two types of systems considered at $T = 1$. Unlike a homogeneous system, where there is a unique function $n_{\xi i} \equiv n_i$ for all sub-volumes, corresponding to a (single) mean field FES parameter α_{eff} , we now have different populations with a spatial distribution. As one can see from Fig. 2 the systems obey a mirrored symmetry: the density of particles in sub-volume ζ drops in the “dip” case and is enhanced in “peak” case, as compared with a mean field calculation for a constant $\sigma = 1.0$. The particle densities in nearest neighbors sub-volumes of ζ , i.e. $\zeta - 1$ and $\zeta + 1$, exhibit deviations from the mean field values and opposite to the values in sub-volume ζ . This can be explained as follows.

At equilibrium, in the case of a dip in the density of states, the repulsive interaction between particles drives accumulations of particles towards the edges of the region with constant $\sigma = 1.0$, as the number of particle in sub-volume ζ is lower due to a smaller number of available states. The opposite is found in the case of a peak in the DOS, where the larger number of particles in sub-volume ζ repel the particles in the adjacent regions. Starting with the $\zeta - 2$, $\zeta + 2$ sub-volumes, the populations already get very close to the mean field values.

However, for dips or peaks of finite widths, a broader distribution of particle densities can be observed in the insets of Fig. 2. Here we took the linear dependences $\sigma_{\zeta+\tau} = \sigma_{\zeta-\tau} = 0.5 + 0.1\tau$ (dip) and $\sigma_{\zeta+\tau} = \sigma_{\zeta-\tau} =$

$2.0 - 0.2\tau$ (peak), with $\tau = 1, 2, 3, 4$. Note that due to the symmetry, except the ζ sub-volume, we have the pairs $\rho_{\zeta-\tau,i} = \rho_{\zeta+\tau,i}$, for any $\tau > 0$.

We further analyze the particle distribution in a periodic one-dimensional system with an interface between high ($\sigma_\xi = 1.0$, for $\xi < N_R/2$) and low ($\sigma_\xi = 0.5$, for $\xi \geq N_R/2$) DOS regions. The obtained results are represented in Fig. 3 for a temperature $T = 1$. From the main plot one can see the particle densities are divided in two groups corresponding to the two values of σ . Like in the previous case, significant deviations occur in the sub-volumes which form the interfaces, which can be understood by a similar reasoning. The particle densities in the other sub-volumes are depicted in detail in the two insets, indicating a convergence towards the values corresponding to the mid-points of the two constant σ regions.

Now we analyze the properties of a system with disorder which we introduce by randomly distributed values for the local density of states σ_ξ at each site. More specifically, we consider a step distribution, centered around the average value $\sigma_0 = 2$ and several degrees of disorder are set by the width of the distribution step $\Delta\sigma$. Figure 4(a) shows a typical particle distribution obtained at a temperature $T = 1$ and maximum disorder, $\Delta\sigma = 4$.

Like in the two previously analyzed examples one can observe the particle densities are larger at sites with larger DOS, although now we find the disorder specific distributions $\rho_{\xi i}$. In the lower plot is represented the local DOS together with the particle distributions at each site ξ , for two temperatures $T_l = 0.5$ and $T_h = 6$. One can see that for the higher temperature T_h the particle distribution follows closely the σ_ξ distribution, while for the lower temperature T_l the particles are more evenly distributed. In the high temperature limit the interactions become less and less important, the particle distributions approach the Maxwell-Boltzmann distribution and all available states become equally probable. Consequently, the spatial particle density ρ_ξ in each sub-volume becomes proportional with the density of states σ_ξ . By contrast, in the lower temperature limit, the repulsive interactions tend to level the particle distribution. At low and intermediate temperatures, there is no clear relation to the local DOS anymore and the exact equilibrium distribution can be obtained using the FES formalism.

The results presented so far for the particle density distributions may be obtained in any of the three descriptions mentioned in the section 2, i.e. the *fermionic*, *bosonic* and *Wu* pictures, which all lead to the same physical results. To further illustrate this fact, we plotted in Fig. 5 the populations and the quasi-particle density of states in the fermionic and bosonic pictures,

for the same disordered system analyzed before ($\sigma_0 = 2$, $\Delta\sigma = 4$, $T = 1$). As expected all the populations in fermionic description, $n_{\xi i}^F$, are smaller than unity, while some of the bosonic populations, $n_{\xi i}^B$, indicate a large increase at low energies. This difference regarding the populations in the two pictures is compensated by the behavior of the quasi-particle density of states, $\tilde{\sigma}^F$ and $\tilde{\sigma}^B$, so that the particle densities $\rho_{\xi i}$ and ρ_{ξ} are the same in any description. Specifically, we have for low energies $\tilde{\sigma}^B < \tilde{\sigma}^F$, while at high energies both $\tilde{\sigma}^B$ and $\tilde{\sigma}^F$ asymptotically approach the Wu density of states, $\tilde{\sigma}^W$.

The heat capacity of such disordered systems exhibits peculiar effects. In a uniform system, i.e. with a constant DOS, the heat capacity is the same for any diagonal FES parameter α [23, 5]. However, here we have FES parameters of the form (13), i.e. diagonal in energy and non-diagonal with respect to position indices. The results are presented in Fig. 6(a) for different distributions of the local DOS, as indicated in the inset, corresponding to the values $\Delta\sigma = 1, 0.75, 0.5\sigma_0$. By increasing the disorder a deviation from the reference constant-DOS dependence of the heat capacity per particle is observed, with a maximum above 1. Similar deviations are observed in the temperature dependence of the entropy in Fig. 6(b), which are in agreement with relation (25). These deviations vanish in the low disorder or high temperature limits.

We also performed ensemble averages on disorder and a qualitatively similar behavior was found.

4. Conclusions

We have formulated an approach based on the fractional exclusion statistics to calculate the thermodynamic properties of disordered interacting systems. The interacting particles are localized at randomly distributed sites in a solid matrix. By partitioning the real space besides the usual division of the energy axis and relating the obtained species by FES parameters we are able to go beyond a mean field picture, describe the particularities of such disordered systems and calculate their thermodynamic properties in an intermediate temperature range.

We also analyzed systems which do not appear to be disordered at the scale at which we partition the system, but exhibit a non-homogeneous distribution of sites. We calculate the particle distributions, the quasiparticle densities of states and we emphasize the margin effects.

Beside its fundamental aspect, this method may be applied in the calculation of the thermodynamic and transport properties of mesoscopic systems.

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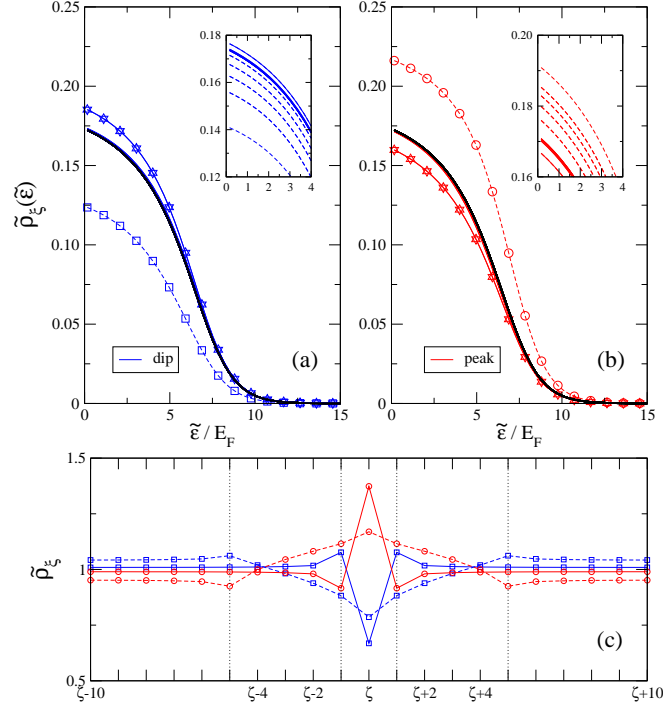


Figure 2: (Color online) Quasiparticle density, $\tilde{\rho}_\xi(\tilde{\epsilon})$, for systems with a *dip* ($\sigma_\zeta = 0.5$) (a) and a *peak* ($\sigma_\zeta = 2.0$) (b) in the otherwise constant density of states ($\sigma_\xi = 1.0$, for $\xi \neq \zeta$). The symbols represent the particle densities which correspond to the species ζ [squares (a) and circles (b)] and its first nearest neighbors (up/down triangles). The solid black lines correspond to a uniform systems with $\sigma = 1.0$. The insets contain similar data for systems with a finite width dip/peak. The dashed lines represent particle densities for sub-volumes $[\zeta - \tau, \zeta + \tau]$, with $\tau \leq 4$. The volume density of (quasi)particles $\tilde{\rho}_\xi$ in each species are represented in (c). Pairs of vertical dotted lines mark the extension of the considered dipoles and peaks.

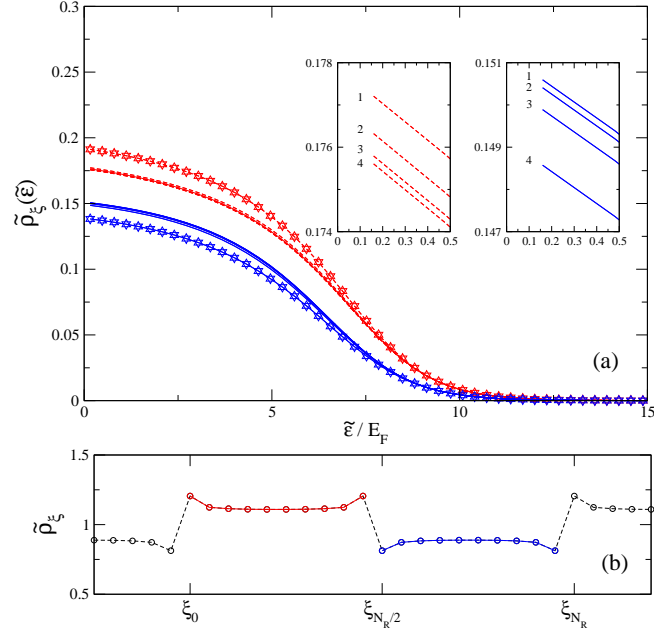


Figure 3: (Color online) (a) Quasiparticle density for a system with a step-like density of states, i.e. $\sigma_\xi = 1$, for $\xi < N_R/2$ (upper curves, in red) and $\sigma_\xi = 0.5$, for $\xi \geq N_R/2$ (lower curves, in blue). The symbols (up/down triangles) correspond to the four sub-volumes located at the interfaces. In the insets (left, for $\xi < N_R/2$, and right, for $\xi \geq N_R/2$) are shown details of $\tilde{\rho}_\xi(\tilde{\epsilon})$ for the remaining sub-volumes. The numbers indicate the minimum distance from either interface. (b) Spatial (quasi)particle density $\tilde{\rho}_\xi$ of the considered system.

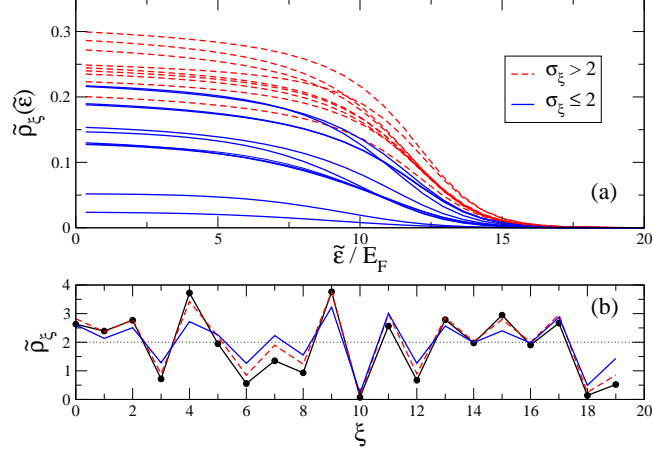


Figure 4: (Color online) (a) Quasiparticle density for a disordered system ($\sigma_0 = 2$, $\Delta\sigma = 4$). The species with high (blue/solid) and low (red/dashed) DOS are indicated. (b) Density of states σ_ξ (black/solid with dots) and particle numbers in each sub-volume for a high ($T_h = 6.0$) (red/dashed) and a low ($T_l = 0.5$) (blue/solid) temperature.

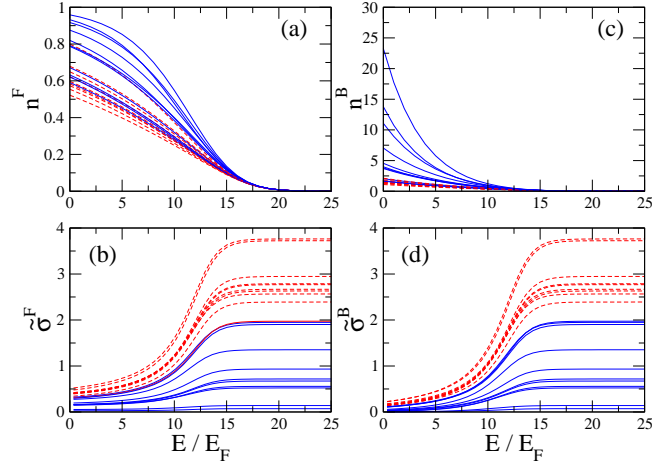


Figure 5: (Color online) Populations and quasi-particle density of states (red/dashed for $\sigma_\xi > 2$, blue/solid for $\sigma_\xi \leq 2$) in the fermionic (a-b) and bosonic (c-d) descriptions.

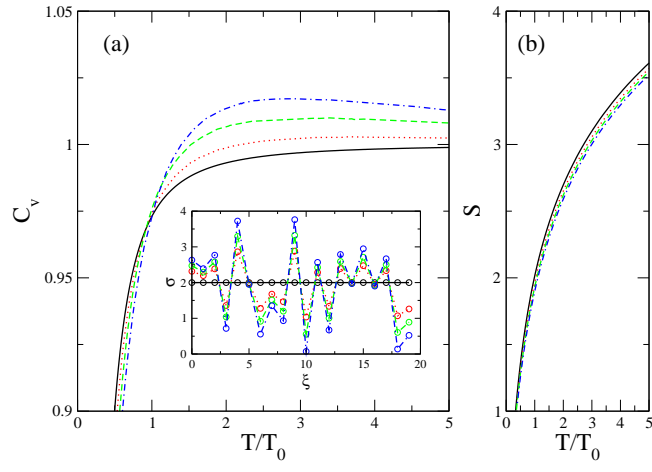


Figure 6: (Color online) Heat capacity (a) and entropy (b) for different degrees of disorder: $\Delta\sigma = 0$ (black/solid), 0.5 (red/dotted), 0.75 (green/dashed) and 1 (blue/dashed-dotted), as indicated in the inset.